Current Capabilities for Generating List-Mode Data for Simulated Subcritical Neutron Measurements Using MCNP*

Avneet Sood, J. Hutchinson, W. Myers, C.J. Solomon, R.C. Little

Los Alamos National Laboratory

Los Alamos, NM 87545

*some material directly taken from previous NCSP talk by B. Little

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Abstract

- **This presentation briefly describes the following topics:**

  - Review of sub-critical multiplication and measurements,
  - Current MCNP simulation capabilities,
  - MCNP modeling needs for comparisons with sub-critical multiplication measurements
  - Summary of FY10 work, Progress on FY11 work

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Many programs are interested in the characterization of these materials:

- **Stockpile Stewardship Program (SSP)**
  - responsible for maintaining the safety, security, and reliability of the nation's nuclear weapons stockpile

- **Nuclear Counter Terrorism (NCT)**
  - identifying and characterizing potential IND material and designs that pose a threat to U.S. citizens, assets, and infrastructure

- **Joint Technical Operations Team (JTOT)**
  - provides specialized technical capabilities in support of lead federal agencies to respond to weapons of mass destruction

- **National Technical Nuclear Forensics (NTNF)**
  - enable operational support for materials, pre-detonation device, and post-detonation nuclear or radiological forensics programs with the broader goal of attribution

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Timeline of Current Effort (1)

- **July 13, 2010 – McKamy asks for Stockpile-Stewardship motivated CEF experiments**

- **August 26, 2010 – Little presents initial ideas during $C_E dT$ meeting in Las Vegas**
  - Reaction-rate ratio experiments
  - High-fidelity re-creation of "gold-standard" assemblies used to set uncertainty 'gates'
  - Experiments for validation of probability-of-initiation calculations
  - Dynamic experiments
  - Alternative materials
  - Experiments with specific reflectors
  - Fission product studies
  - Production of radioactive samples for NTNF exercises
  - Source for INRAD studies
  - High-resolution leakage spectra (neutrons and gammas)
  - Tailored neutron spectra
  - Experiments driven by 14-MeV neutron source
  - New assemblies used as "blind exercises" for ASC codes / physics / designers

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Timeline of Current Effort (2)

- **September – October, 2010**
  - LANL determined "top-3" experiments and submitted IERs
  - Obtained LLNL concurrence (thank you!)

- **November 8, 2010 – Ellis' $C_E dT$ meeting during ANS**
  - Titles provided for additional IERs

- **January 26, 2011 – NCT / NCSP Neutronics Roadmap Meeting at LLNL**
  - Discussion of LANL / LLNL NCT priorities for CEF experiments
  - Six IERs identified as top priorities
  - Results communicated to NCSP Management Team

- **January - February 2011**
  - LANL submits 8 additional IERs in support of stockpile stewardship and global security programs

- **15 June 2011: Planet goes critical!**

Key Objectives Common to Submitted IERs

- **Benchmark Quality**
  - Material characterization
  - Assembly details
  - Experimental environment

- **Focus on Uncertainties**
  - While planning, performing, and documenting the experiment
  - Uncertainties are as important as the mean!

- **Multiple Critical Configurations**
  - To determine reproducibility
  - With various reflectors to modify neutron spectrum

- **Examine More than Critical Configuration**
  - Sub-critical and super-critical
  - External neutron and gamma spectra
  - Internal foils and detectors to measure reaction rates and reaction products

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The goal of our simulations is to be predictive!

- **MCNP – well suited for comparing results of sub-critical measurements**
  - Calculates relevant quantities for fixed-source, eigenvalue problems
    - How faithfully is MCNP simulating fission process and what we measure?
    - Correct for averaged values but **not microscopically correct**

- **Other MCNP-like capabilities exist:**
  - MCNP-PoliMi
  - MCNP-DSP
  - Others?
  - We are currently evaluating these capabilities.

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Relevant Physics for Sub-Critical Multiplication

- **(Source) Passive neutrons from fissionable material emitted from:**
  - Spontaneous fission neutron sources:
    - Correlated in time and location of fission
    - Examples: Cf-252, Pu-240
  - (α,n) reactions:
    - Produced when α particle is absorbed and neutron is emitted
    - Not correlated in time and location
    - Examples: Am-Be

- **(Induced) Neutron multiplication dominated by two physical processes:**
  - (n,2n)
    - Occurs mostly above 7 MeV
    - Does not contribute significantly to most scenarios
  - Neutron-induced Fission

> Simulations need to be "microscopically" correct for comparisons with measured data.

Sub-critical Measurements

- **Neutron multiplication measurements (passive and active) designed to separate the correlated emission events, e.g., SF, from the uncorrelated events, e.g. , (α,n),**
  - Record time of neutron capture in a neutron detector over a large collection time (e.g. 300 sec)
  - Group these capture times in a large number (e.g. 1 M) smaller time sub-intervals (e.g. 250 μsec)
    - These time sub-intervals are larger than typical neutron detection and lifetimes (~50 μsec)
  - Multiplicity histogram is constructed
    - Obeys Poisson statistics if system is non-multiplying (i.e. neutrons are emitted randomly in time)
    - Data analysis begins…Feynman Variance-to-Mean, CSDNA, etc

Data recorded is neutron detector location and time: list-mode data

Simulations need to produce list-mode data for comparisons

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MCNP Simulations of Sub-Critical Measurement

- **MCNP simulation of neutron sources and detection**
  - User can define location, direction, energy, time, and intensity of SF, (α,n) neutron sources
  - User **<u>cannot</u>** define fission events
    - e.g. sample number of neutrons emitted from ν_{bar}
  - User **<u>cannot</u>** define correlated (time, location) neutron sources
    - MCNP samples these values from user's input
  - User <u>cannot</u> (easily) record location and time of detection.
    - Possible using MCNP's PTRAC capability and a user-created external script to extract this information

Standard MCNP is not microscopically correct enough to compare with current sub-critical measurements:

FY10 Proposal to NCSP

- **Upgrade an existing (unreleased) capability for MCNP**
  - Use of Terrell (Lestone - new) data to statistically sample the actual number of neutrons ν released when induced fissions occurred in a calculation.
    - MCNP can do this for <u>induced fissions, but not starting sources</u>
  - Add capability to have a fixed source problem that started fission events (correlated) rather than individual neutron histories (independent samples),
  - Add capability to allow for a non-fissioning interrogating source (eg. AmBe), and
  - Add capability to write a special output file that contained the location and time at which each neutron was captured (list-mode data)
  - <u>Resulting list-mode data can be evaluated by any analysis technique</u>
  - **Capability has existed separately for over 25 years (internally V&V'd)**
  - **Difficult to maintain separately**
    - Make use of MCNP's user-defined subroutines SOURCE/TALLYX
    - Compare to existing benchmarks

- **FY10 proposal leveraged on-going experiments and equipment improvements to record list-mode data (e.g. PATRM/PMC)**

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Deliverables for FY10

- **(1) Update the list-mode/fission source capability to current MCNP.**
  - Implement this capability as a routine that can be applied to any future version of MCNP through the SOURCEX and TALLYX routines provided with MCNP.
  - Produce MCNP5.1.51 executable (sequential, OpenMPI) with standard features plus correlated sources and list-mode capability.

- **(2) Compare and document simulated results with previous experimental results performed.**

- **(3) Compare and document simulated results with experiments to be performed at LANL or other ICSBEP experiments**
  - (a,n) sources with poly, SS shells, etc
  - SUB-PU-MET-FAST-001,002,and 003

- **(4) Begin R&D for application of variance reduction techniques to accelerate convergence of problems (current simulations are performed in analog mode)**

- **(5) Compare and document our simulation results using currently available codes MCNP-DSP and MCNP-Polimi (code-to-code verification)**
  - UNLV sub-task

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FY10 Q4 Results

- **Internally-developed multiplication patch to MCNP has been updated to current version of MCNP**
  - Coding existed in internal (much older) version of MCNP
  - Initial testing indicates code is working as expected. Comparison with experiments begun.
  - Still working on developing an independent SOURCE and TALLYX subroutine

- **Validation experiments performed at NTS/DAF**
  - Diagnostics included 2 NPODS, SNAP, 140% HPGe.
    - List-mode data taken, MCNP models developed/improved
  - **May 2010:** BeRP ball (bare), BeRP ball moderated with increasingly thick shells, BeRP ball moderated with fixed outer dimension and variable thickness
    - BeRP ball supported with hemi-shell – no longer a 1-D problem!
    - Two different moderators
  - **July 2010:** BeRP with different moderator, Active interrogation with D-T source
  - **September 2010:** Rocky Flat Shells (HEU) with Cf-252 source and multiple poly configurations

FY11 Q1 - progress

- **SOURCE/TALLYX subroutines written**
  - Subroutines intended for user-defined source and tally
  - Independent of MCNP – no modification of MCNP is required
  - Works with MCNP5.1.60 (current release)

- **SOURCE—modifies definition of starting particle to be a starting reaction, e.g., spontaneous fission, samples starting particles from that reaction**

- **TALLYX—modifies a type 4 tally to produce a file of absorption times in tally cell, a.k.a. list-mode data**

- **Tally output can be processed to analyze inferred multiplication**

> We plan to submit SOURCE/TALLYX routines to MCNP code development team for adaptation into MCNP6 with documentation, validation benchmarks, etc

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SOURCE Input Uses RDUM Card

- **Input for the source is specified on the RDUM card**

  EXAMPLE:

```
RDUM    1000  94240  10000    1    2    1    0.0   0.0   0.0    3
```

Cell # of starting reaction

SF ZAID

# of reactions to start

ERG dist #

TME dist #

Spatial sampling method

POS

RAD dist #

- **Multiple cells and SF ZAID combinations may be specified—sampled based on the # of starting reactions**

Tally Modification Requires FU Card

- **The FU card modifies the tally to score captures**

- **Requires analog simulation**
  - Sample induced fission multiplicity

  `phys:n 4j  1` or `phys:n  4j  2`
  - Turn off default implicit capture

  `cut:n  2j  0`

- **EXAMPLE:**

```
F4:n  1001  $ Tally on cell 4

FU4  2003  $ Score captures by ZAID 2003 (He-3)
```

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Example Tally List-Mode Output

```
3050        2902347683.93636
3049       25617701923.43888
3052       28074609346.68214
3050       20857333210.41721
3052       16140211088.86106
3053       24770874466.83554
3047       24759462750.29287
3049       15567786730.17038
3052       21217419855.78508
3052       21217402172.59257
3061       21217406407.25473
3048       21217404433.38023
3049        5437041302.96633
```

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Ongoing Validation Measurements at DAF

- **WGPu**
  - Berp ball with different moderators
  - Measurements are done, simulations are in progress

- **HEU**
  - Rocky Flats shells with different moderators and interrogating sources (SF, (a,n))
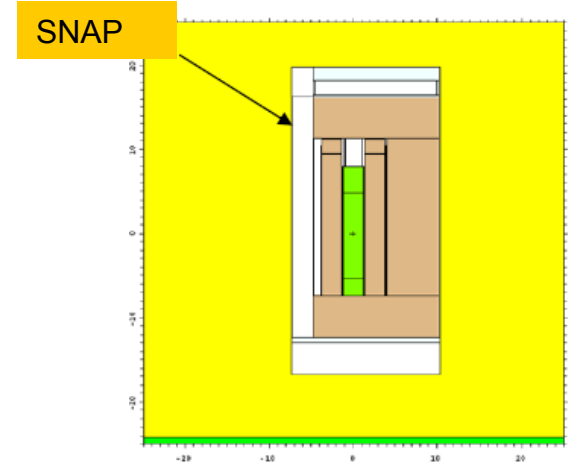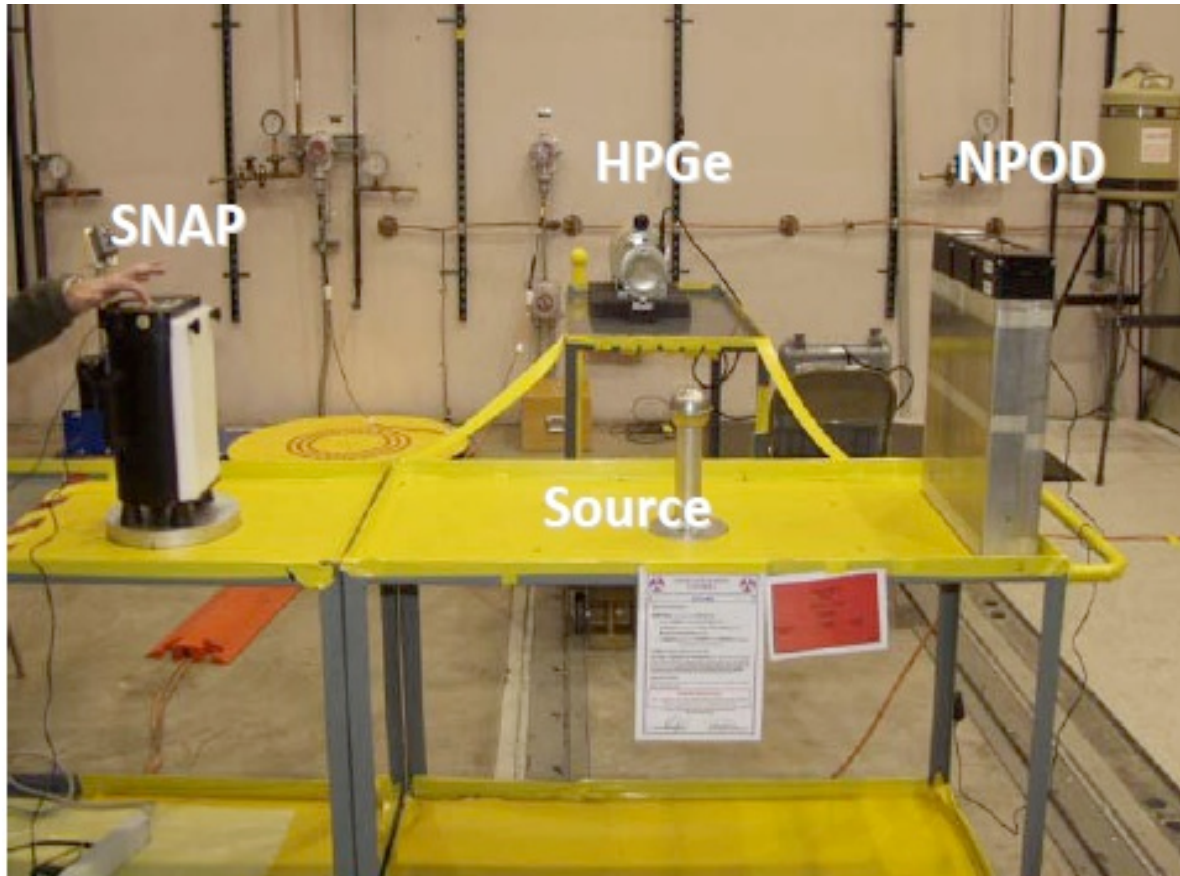 - Measurements are done, simulations are in progress
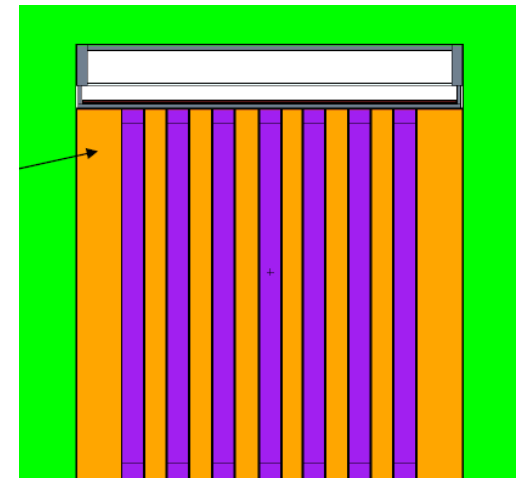
- **SF and (a,n) Sources:**
  - Multiple moderators

- **Active Sources**
  - D-T generator source
  - WGPu, HEU
  - Measurements are done, simulations are in progress

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1st "Benchmark" Comparison: SNL - SINBAD

SNAP

HPGe

NPOD

SNAP

NPOD-3

- J. Mattingly, "Polyethylene-Reflected Pu metal Sphere," SAND2009-5804

Status and Future of NCSP Work

- **FY11 proposed work:**
  - Continue comparison of MCNP simulations' list-mode output to relevant sub-critical benchmark experiments for code validation
  - Simultaneously we wish to perform neutron leakage and neutron spectra measurements for additional points of comparison for our MCNP list-mode simulations.
    - Comparison of non-integral results for same neutron sources/scattering environments will give further confidence in the MCNP simulation results
    - Additional measurements will allow us to characterize room return as well as determine neutron detector efficiency.

Extra

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Specific Objectives of Proposed Experiments (1)

- **Reaction rate and fission-product yield measurements in Pu-239 and U-238,235**

  - Address known deficiencies in our current understanding of fission chain yields in various neutron spectra

  - Reestablish experimental capability (radiochemistry and nuclear physics) relevant to stewardship and NTNF

  - Note that several LANL radiochemists are planning to tour CEF in March (hosted by John Bounds) to better understand ancillary capabilities at CEF and to prepare for initial experiment.

- **Probability of Initiation Benchmark Experiments**

  - Develop a set of documented experimental data that is specifically designed to test our ability to compute the probability of initiating a divergent neutron chain reaction

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Specific Objectives of Proposed Experiments (2)

- **Measure the Fission Neutron Spectrum Shape Using Threshold Activation Detectors**

  - We propose to measure reaction rates on several threshold detectors in different regions (spectra) of critical assemblies to reduce the current uncertainty in the shape and magnitude of the high-energy tail of the prompt neutron fission spectrum.

  - This experiment would complement ongoing theory improvements and the "Chi-Nu" detector system being constructed at LANSCE that will measure the PNFS tails directly.

- **Be Reflector Studies**

  - There is a need to resolve the fact that existing suites of ICSBEP HEU-Be systems (HMF58, HMF66, and HMF77) have inconsistent C/E ratios based on ENDF/B-VII.0

  - This experiment would build on IER 137, and would complement updated R-Matrix evaluation work and RPI scattering experiments on Be-9.